



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 14, 2017 – 06:53 am GMT

PDB ID : 2AKM  
Title : Fluoride Inhibition of Enolase: Crystal Structure of the Inhibitory Complex  
Authors : Qin, J.; Chai, G.; Brewer, J.M.; Lovelace, L.L.  
Deposited on : 2005-08-03  
Resolution : 1.92 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : 1.9-1692  
EDS : trunk28620  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : recalc28949

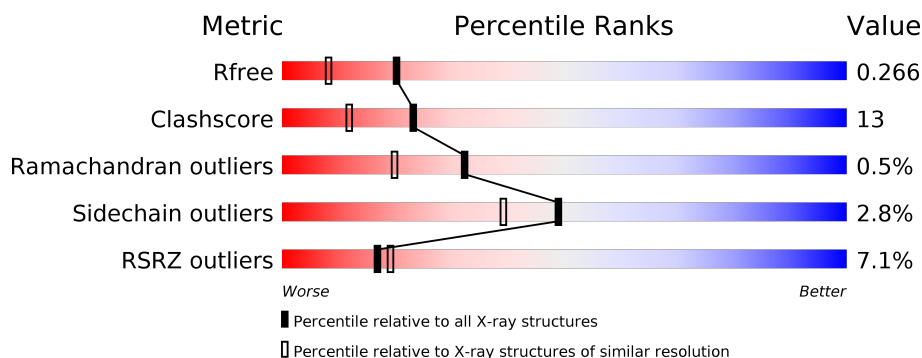
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.92 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	100719	6276 (1.94-1.90)
Clashscore	112137	7025 (1.94-1.90)
Ramachandran outliers	110173	6947 (1.94-1.90)
Sidechain outliers	110143	6948 (1.94-1.90)
RSRZ outliers	101464	6332 (1.94-1.90)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	439	<div> <div>9%</div> <div> <div></div> <div>75%</div> <div>22%</div> <div>..</div> </div> </div>
1	B	439	<div> <div>5%</div> <div> <div></div> <div>74%</div> <div>22%</div> <div>..</div> </div> </div>

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 6948 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Gamma enolase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	433	Total	C	N	O	S	0	0	0
			3273	2066	557	637	13			
1	B	432	Total	C	N	O	S	0	0	0
			3277	2065	560	639	13			

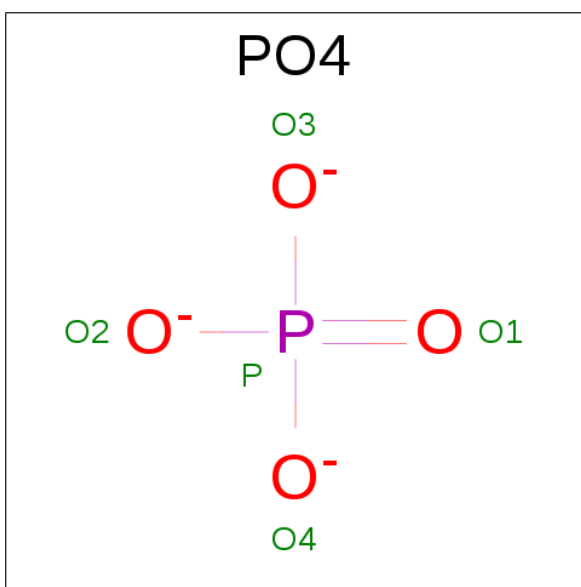
There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	434	HIS	-	EXPRESSION TAG	UNP P09104
A	435	HIS	-	EXPRESSION TAG	UNP P09104
A	436	HIS	-	EXPRESSION TAG	UNP P09104
A	437	HIS	-	EXPRESSION TAG	UNP P09104
A	438	HIS	-	EXPRESSION TAG	UNP P09104
A	439	HIS	-	EXPRESSION TAG	UNP P09104
B	434	HIS	-	EXPRESSION TAG	UNP P09104
B	435	HIS	-	EXPRESSION TAG	UNP P09104
B	436	HIS	-	EXPRESSION TAG	UNP P09104
B	437	HIS	-	EXPRESSION TAG	UNP P09104
B	438	HIS	-	EXPRESSION TAG	UNP P09104
B	439	HIS	-	EXPRESSION TAG	UNP P09104

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

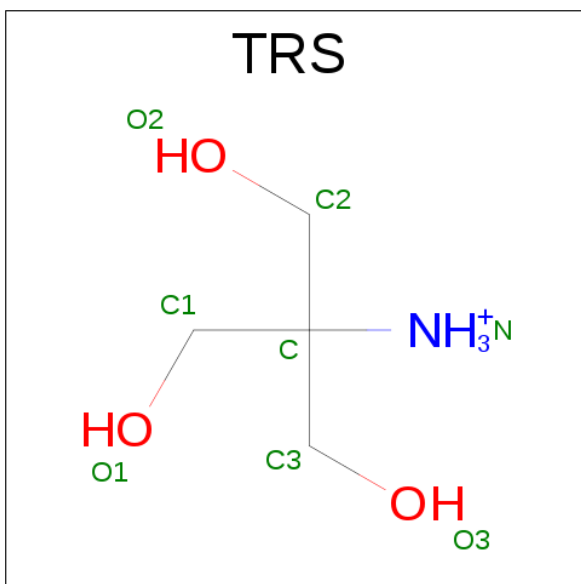
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	Mg	0	0
			1	1		
2	A	2	Total	Mg	0	0
			2	2		

- Molecule 3 is PHOSPHATE ION (three-letter code: PO4) (formula: O<sub>4</sub>P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	P	0	0
			5	4	1		
3	B	1	Total	O	P	0	0
			5	4	1		

- Molecule 4 is 2-AMINO-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (three-letter code: TRS) (formula:  $C_4H_{12}NO_3$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			8	4	1	3		

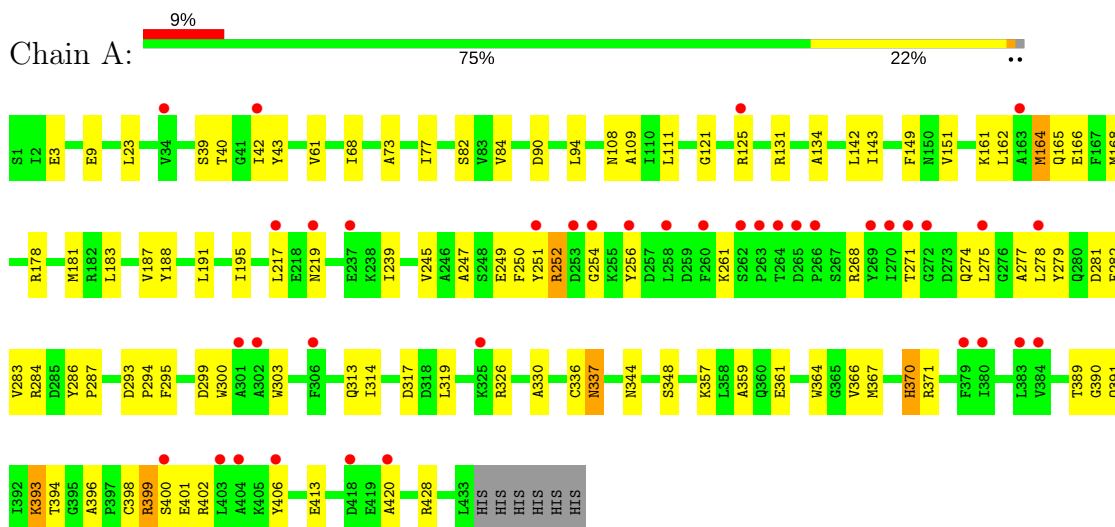
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	186	Total 186	O 186	0	0
5	B	191	Total 191	O 191	0	0

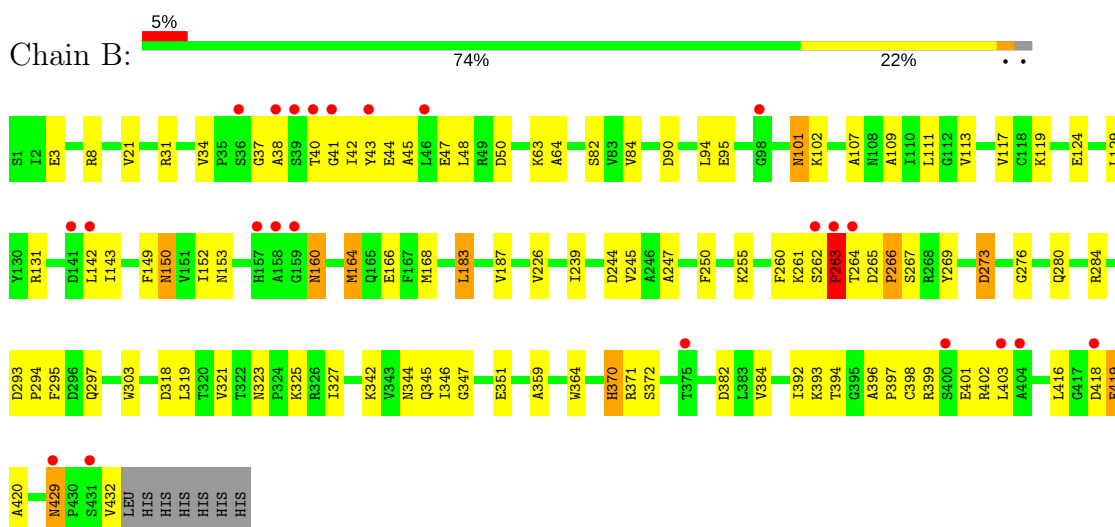
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

#### • Molecule 1: Gamma enolase



#### • Molecule 1: Gamma enolase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	111.74Å 119.69Å 68.30Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 1.92 41.75 – 1.92	Depositor EDS
% Data completeness (in resolution range)	74.7 (50.00-1.92) 74.8 (41.75-1.92)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.52 (at 1.92Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.211 , 0.249 0.230 , 0.266	Depositor DCC
$R_{free}$ test set	2649 reflections (5.02%)	DCC
Wilson B-factor (Å <sup>2</sup> )	19.7	Xtriage
Anisotropy	1.058	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 50.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.45$ , $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	6948	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.14% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: TRS, MG, PO4

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	A	0.37	1/3328 (0.0%)	0.57	0/4509
1	B	0.38	1/3332 (0.0%)	0.58	0/4513
All	All	0.38	2/6660 (0.0%)	0.58	0/9022

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	3	GLU	CD-OE2	7.17	1.33	1.25
1	B	3	GLU	CD-OE2	6.82	1.33	1.25

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3273	0	3208	81	0
1	B	3277	0	3225	88	0
2	A	2	0	0	0	0
2	B	1	0	0	0	0
3	A	5	0	0	0	0
3	B	5	0	0	1	0
4	A	8	0	12	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	A	186	0	0	6	0
5	B	191	0	0	8	0
All	All	6948	0	6445	167	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 13.

All (167) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:273:ASP:HB3	5:B:533:HOH:O	1.81	0.80
1:B:429:ASN:N	1:B:429:ASN:HD22	1.84	0.75
1:B:429:ASN:H	1:B:429:ASN:HD22	1.34	0.73
1:B:342:LYS:NZ	3:B:442:PO4:O2	2.18	0.72
1:B:40:THR:HG22	1:B:371:ARG:HH12	1.56	0.70
1:B:131:ARG:HE	1:B:142:LEU:HD11	1.58	0.69
1:A:164:MET:HB2	1:A:219:ASN:ND2	2.09	0.68
1:A:40:THR:HG22	1:A:371:ARG:HH22	1.59	0.67
1:A:293:ASP:OD2	1:A:317:ASP:HB3	1.95	0.67
1:A:111:LEU:HD22	1:A:344:ASN:HA	1.78	0.65
1:A:357:LYS:O	1:A:361:GLU:HG3	1.96	0.65
1:A:250:PHE:HA	1:A:252:ARG:HH21	1.62	0.65
1:A:261:LYS:HB2	5:A:505:HOH:O	1.96	0.64
1:B:84:VAL:HG13	1:B:124:GLU:HG2	1.80	0.63
1:A:268:ARG:HG3	1:A:268:ARG:HH21	1.64	0.62
1:A:165:GLN:HG2	1:A:166:GLU:HG3	1.81	0.62
1:B:34:VAL:HG13	1:B:111:LEU:HD23	1.81	0.62
1:A:142:LEU:HD22	1:A:142:LEU:H	1.65	0.62
1:A:393:LYS:O	1:A:393:LYS:HG3	2.00	0.61
1:A:247:ALA:HA	1:A:250:PHE:CE1	2.36	0.60
1:B:342:LYS:HB2	1:B:345:GLN:HE21	1.67	0.60
1:B:101:ASN:H	1:B:101:ASN:HD22	1.49	0.59
1:B:266:PRO:HA	1:B:269:TYR:CE2	2.37	0.59
1:A:68:ILE:HD11	1:A:109:ALA:HA	1.84	0.59
1:A:281:ASP:HA	1:A:284:ARG:HH11	1.67	0.59
1:B:152:ILE:HD12	1:B:226:VAL:HG23	1.84	0.58
1:B:342:LYS:HB2	1:B:345:GLN:NE2	2.19	0.57
1:B:44:GLU:HB3	1:B:345:GLN:HG2	1.86	0.57
1:B:94:LEU:CD2	1:B:102:LYS:HE3	2.35	0.57
1:B:164:MET:HG2	1:B:245:VAL:HG22	1.85	0.57
1:A:143:ILE:HD11	1:A:390:GLY:HA2	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:367:MET:HA	1:A:391:GLN:HG3	1.86	0.56
1:B:143:ILE:HD12	1:B:143:ILE:O	2.04	0.56
1:A:247:ALA:HA	1:A:250:PHE:CZ	2.40	0.56
1:B:359:ALA:O	1:B:364:TRP:HB2	2.05	0.56
1:B:41:GLY:O	1:B:44:GLU:HG2	2.06	0.56
1:A:314:ILE:H	1:A:337:ASN:HD21	1.54	0.55
1:A:151:VAL:HG12	1:A:188:TYR:HD1	1.71	0.55
1:A:398:CYS:O	1:A:399:ARG:HB2	2.07	0.55
1:B:82:SER:OG	1:B:84:VAL:HG22	2.06	0.55
1:A:279:TYR:O	1:A:283:VAL:HG23	2.07	0.55
1:A:181:MET:CE	1:A:406:TYR:HB3	2.36	0.55
1:B:398:CYS:O	1:B:399:ARG:HB2	2.07	0.55
1:A:300:TRP:HZ2	1:A:326:ARG:NH2	2.05	0.55
1:B:64:ALA:HB1	1:B:109:ALA:HB2	1.89	0.54
1:A:400:SER:OG	1:B:401:GLU:HB3	2.08	0.54
1:B:131:ARG:HG3	1:B:131:ARG:HH21	1.72	0.54
1:A:164:MET:HG3	1:A:245:VAL:HG13	1.88	0.53
1:A:161:LYS:HB3	1:A:217:LEU:HD13	1.89	0.53
1:B:90:ASP:O	1:B:94:LEU:HG	2.08	0.53
1:B:101:ASN:N	1:B:101:ASN:HD22	2.06	0.53
1:B:160:ASN:HD22	1:B:261:LYS:HZ2	1.54	0.53
1:A:9:GLU:HG3	1:A:61:VAL:CG2	2.39	0.53
1:A:42:ILE:HG13	1:A:43:TYR:CD1	2.44	0.52
1:B:247:ALA:HA	1:B:250:PHE:CE1	2.45	0.52
1:B:344:ASN:OD1	1:B:371:ARG:NH2	2.41	0.52
1:A:90:ASP:O	1:A:94:LEU:HG	2.10	0.52
1:B:293:ASP:HA	1:B:303:TRP:CH2	2.45	0.51
1:B:113:VAL:O	1:B:117:VAL:HG23	2.09	0.51
1:A:300:TRP:CZ2	1:A:326:ARG:NH2	2.78	0.51
1:B:429:ASN:ND2	1:B:429:ASN:N	2.57	0.51
1:B:160:ASN:ND2	1:B:261:LYS:HZ2	2.10	0.50
1:B:95:GLU:HG3	5:B:566:HOH:O	2.10	0.50
1:B:346:ILE:HG12	1:B:351:GLU:HB3	1.94	0.50
1:A:191:LEU:O	1:A:195:ILE:HG13	2.11	0.50
1:B:164:MET:CG	1:B:245:VAL:HG22	2.41	0.50
1:A:295:PHE:HB2	1:A:303:TRP:NE1	2.27	0.50
1:B:250:PHE:HB3	1:B:260:PHE:CD2	2.46	0.50
1:B:111:LEU:HD22	1:B:344:ASN:HA	1.94	0.50
1:B:284:ARG:HG2	5:B:519:HOH:O	2.12	0.49
1:A:370:HIS:CD2	1:A:370:HIS:H	2.29	0.49
1:A:9:GLU:HG3	1:A:61:VAL:HG22	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:313:GLN:HA	1:A:337:ASN:HD21	1.76	0.49
1:A:142:LEU:HD22	1:A:142:LEU:N	2.27	0.49
1:A:40:THR:HG22	1:A:371:ARG:NH2	2.26	0.48
1:B:131:ARG:HG3	1:B:131:ARG:NH2	2.28	0.48
1:A:268:ARG:HG3	1:A:268:ARG:NH2	2.27	0.48
1:A:149:PHE:O	1:A:168:MET:HA	2.14	0.48
1:B:149:PHE:O	1:B:168:MET:HA	2.13	0.48
1:B:50:ASP:HA	1:B:63:LYS:HD2	1.96	0.48
1:B:393:LYS:O	1:B:393:LYS:HG3	2.14	0.48
1:B:47:GLU:HB3	5:B:493:HOH:O	2.13	0.48
1:A:314:ILE:H	1:A:337:ASN:ND2	2.11	0.48
1:A:178:ARG:HD2	5:A:643:HOH:O	2.15	0.47
1:B:160:ASN:ND2	1:B:261:LYS:NZ	2.62	0.47
1:B:43:TYR:HB2	1:B:321:VAL:HG21	1.97	0.47
1:A:164:MET:H	1:A:219:ASN:HD21	1.61	0.47
1:B:131:ARG:NE	1:B:142:LEU:HD11	2.27	0.47
1:B:370:HIS:O	1:B:371:ARG:HD2	2.14	0.47
1:B:43:TYR:HA	5:B:492:HOH:O	2.15	0.46
1:A:121:GLY:O	1:A:125:ARG:HG3	2.16	0.46
1:A:277:ALA:HB2	5:A:548:HOH:O	2.15	0.46
1:B:255:LYS:HB3	1:B:269:TYR:HB3	1.97	0.46
1:B:396:ALA:HB1	1:B:397:PRO:HD2	1.97	0.46
1:A:82:SER:HB3	1:A:84:VAL:HG22	1.98	0.46
1:B:150:ASN:O	1:B:396:ALA:HB2	2.16	0.46
1:A:165:GLN:HG2	1:A:166:GLU:CG	2.46	0.46
1:A:43:TYR:HD1	5:A:514:HOH:O	1.99	0.46
1:B:48:LEU:HD12	5:B:553:HOH:O	2.16	0.46
1:A:428:ARG:HB2	5:A:606:HOH:O	2.14	0.45
1:B:37:GLY:HA2	1:B:371:ARG:HB3	1.98	0.45
1:B:44:GLU:CB	1:B:345:GLN:HG2	2.46	0.45
1:B:384:VAL:HG21	1:B:392:ILE:HB	1.98	0.45
1:B:294:PRO:HD2	1:B:303:TRP:CH2	2.51	0.45
1:B:183:LEU:HD23	1:B:183:LEU:N	2.32	0.45
1:B:303:TRP:CE3	1:B:319:LEU:HD22	2.52	0.45
1:A:401:GLU:CG	1:A:402:ARG:NE	2.80	0.45
1:B:119:LYS:HD3	5:B:601:HOH:O	2.16	0.45
1:B:418:ASP:C	1:B:420:ALA:H	2.20	0.45
1:B:276:GLY:O	1:B:280:GLN:HG2	2.17	0.44
1:A:300:TRP:HZ3	1:A:330:ALA:HA	1.83	0.44
1:A:299:ASP:OD1	1:A:299:ASP:O	2.34	0.44
1:B:37:GLY:HA3	1:B:371:ARG:CZ	2.47	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:161:LYS:O	1:A:162:LEU:C	2.56	0.44
1:B:166:GLU:HB2	1:B:244:ASP:HB3	1.99	0.44
1:A:370:HIS:ND1	1:A:402:ARG:NH1	2.63	0.44
1:A:366:VAL:O	1:A:389:THR:HB	2.18	0.44
1:B:164:MET:HG3	1:B:245:VAL:HG13	2.00	0.44
1:B:129:LEU:HB3	1:B:382:ASP:OD2	2.18	0.44
1:A:400:SER:CB	1:B:401:GLU:HB3	2.48	0.44
1:A:314:ILE:O	1:A:336:CYS:HB2	2.18	0.43
1:B:295:PHE:HB2	1:B:303:TRP:CD1	2.53	0.43
1:B:43:TYR:HD1	5:B:586:HOH:O	2.01	0.43
1:A:401:GLU:HG2	1:A:402:ARG:NE	2.33	0.43
1:B:370:HIS:CG	1:B:394:THR:HA	2.54	0.43
1:A:39:SER:HA	1:A:249:GLU:OE1	2.17	0.43
1:A:23:LEU:HD23	1:A:23:LEU:C	2.38	0.43
1:A:108:ASN:N	1:A:108:ASN:OD1	2.52	0.43
1:B:84:VAL:CG1	1:B:124:GLU:HG2	2.47	0.42
1:A:134:ALA:HB2	1:A:142:LEU:HD11	2.01	0.42
1:A:413:GLU:HG3	1:A:420:ALA:HB1	2.00	0.42
1:B:429:ASN:O	1:B:432:VAL:HG22	2.19	0.42
1:A:278:LEU:HG	1:A:282:PHE:CZ	2.55	0.42
1:B:187:VAL:HG21	1:B:239:ILE:CD1	2.49	0.42
1:B:152:ILE:CD1	1:B:226:VAL:HG23	2.49	0.42
1:A:178:ARG:HB2	5:A:643:HOH:O	2.18	0.42
1:A:183:LEU:O	1:A:187:VAL:HG23	2.19	0.42
1:B:403:LEU:HA	1:B:403:LEU:HD13	1.80	0.42
1:A:367:MET:SD	1:A:393:LYS:HG2	2.59	0.42
1:A:73:ALA:O	1:A:77:ILE:HG13	2.19	0.42
1:B:45:ALA:HB1	1:B:107:ALA:HB2	2.01	0.42
1:B:262:SER:O	1:B:263:PRO:C	2.58	0.42
1:A:300:TRP:HZ2	1:A:326:ARG:HH21	1.67	0.41
1:B:265:ASP:O	1:B:267:SER:N	2.53	0.41
1:A:396:ALA:C	1:A:398:CYS:H	2.23	0.41
1:B:42:ILE:HG12	1:B:297:GLN:OE1	2.21	0.41
1:A:251:TYR:OH	1:A:254:GLY:HA2	2.20	0.41
1:B:143:ILE:HD12	1:B:143:ILE:C	2.41	0.41
1:B:394:THR:O	1:B:402:ARG:HB3	2.21	0.41
1:A:303:TRP:CE3	1:A:319:LEU:HD22	2.56	0.41
1:A:370:HIS:CG	1:A:394:THR:HA	2.56	0.41
1:B:416:LEU:O	1:B:419:GLU:HG3	2.21	0.41
1:A:256:TYR:CD2	1:A:275:LEU:HD22	2.56	0.41
1:A:294:PRO:HD2	1:A:303:TRP:CH2	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:346:ILE:HG23	1:B:347:GLY:N	2.35	0.41
1:A:271:THR:H	1:A:274:GLN:NE2	2.19	0.41
1:A:165:GLN:NE2	1:A:166:GLU:OE2	2.54	0.40
1:A:178:ARG:HG2	1:A:178:ARG:HH21	1.86	0.40
1:A:286:TYR:HB3	1:A:287:PRO:HD2	2.03	0.40
1:B:323:ASN:HD21	1:B:325:LYS:HE3	1.86	0.40
1:A:131:ARG:NH1	1:A:142:LEU:HD21	2.35	0.40
1:B:160:ASN:HD22	1:B:160:ASN:C	2.25	0.40
1:B:38:ALA:HB2	1:B:372:SER:OG	2.21	0.40
1:B:21:VAL:O	1:B:31:ARG:HA	2.21	0.40
1:B:323:ASN:O	1:B:327:ILE:HG13	2.21	0.40
1:A:183:LEU:HB3	1:A:239:ILE:HD11	2.02	0.40
1:A:359:ALA:O	1:A:364:TRP:HB2	2.21	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	431/439 (98%)	401 (93%)	29 (7%)	1 (0%)	51	41
1	B	430/439 (98%)	398 (93%)	29 (7%)	3 (1%)	25	13
All	All	861/878 (98%)	799 (93%)	58 (7%)	4 (0%)	32	20

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	263	PRO
1	B	266	PRO
1	B	419	GLU
1	A	399	ARG

### 5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	335/356 (94%)	329 (98%)	6 (2%)	64	59
1	B	339/356 (95%)	326 (96%)	13 (4%)	38	26
All	All	674/712 (95%)	655 (97%)	19 (3%)	49	39

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	164	MET
1	A	252	ARG
1	A	337	ASN
1	A	348	SER
1	A	370	HIS
1	A	393	LYS
1	B	8	ARG
1	B	101	ASN
1	B	150	ASN
1	B	153	ASN
1	B	160	ASN
1	B	164	MET
1	B	183	LEU
1	B	263	PRO
1	B	264	THR
1	B	273	ASP
1	B	318	ASP
1	B	370	HIS
1	B	429	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	54	GLN
1	A	135	GLN
1	A	150	ASN

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Mol	Chain	Res	Type
1	A	189	HIS
1	A	215	ASN
1	A	219	ASN
1	A	309	ASN
1	A	337	ASN
1	A	360	GLN
1	A	426	ASN
1	B	91	ASN
1	B	101	ASN
1	B	150	ASN
1	B	153	ASN
1	B	160	ASN
1	B	323	ASN
1	B	345	GLN
1	B	429	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 6 ligands modelled in this entry, 3 are monoatomic - leaving 3 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	PO4	A	442	2	4,4,4	1.41	0	6,6,6	0.38	0
4	TRS	A	460	-	7,7,7	0.98	0	9,9,9	2.60	4 (44%)
3	PO4	B	442	-	4,4,4	1.34	0	6,6,6	0.38	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	PO4	A	442	2	-	0/0/0/0	0/0/0/0
4	TRS	A	460	-	-	0/9/9/9	0/0/0/0
3	PO4	B	442	-	-	0/0/0/0	0/0/0/0

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	460	TRS	C1-C-N	-2.84	101.68	107.73
4	A	460	TRS	O2-C2-C	2.55	117.86	110.47
4	A	460	TRS	O1-C1-C	4.24	122.74	110.47
4	A	460	TRS	C2-C-N	5.00	118.35	107.73

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	442	PO4	1	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.



## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	433/439 (98%)	0.66	38 (8%) 11 12	17, 33, 60, 71	0
1	B	432/439 (98%)	0.40	23 (5%) 27 31	17, 31, 53, 75	0
All	All	865/878 (98%)	0.53	61 (7%) 17 19	17, 32, 57, 75	0

All (61) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	260	PHE	5.8
1	B	263	PRO	4.6
1	A	264	THR	4.4
1	A	266	PRO	4.4
1	A	217	LEU	4.1
1	B	159	GLY	3.9
1	A	275	LEU	3.7
1	B	264	THR	3.6
1	A	380	ILE	3.6
1	A	406	TYR	3.5
1	B	142	LEU	3.5
1	A	278	LEU	3.5
1	B	46	LEU	3.4
1	B	41	GLY	3.4
1	A	263	PRO	3.3
1	A	418	ASP	3.2
1	A	251	TYR	3.2
1	B	38	ALA	3.1
1	A	404	ALA	3.1
1	A	269	TYR	3.0
1	A	403	LEU	3.0
1	B	43	TYR	3.0
1	B	40	THR	2.9
1	A	42	ILE	2.8

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Mol	Chain	Res	Type	RSRZ
1	B	141	ASP	2.8
1	A	271	THR	2.8
1	A	163	ALA	2.7
1	A	270	ILE	2.7
1	A	256	TYR	2.7
1	B	262	SER	2.7
1	A	265	ASP	2.6
1	B	36	SER	2.6
1	A	253	ASP	2.5
1	A	258	LEU	2.5
1	A	301	ALA	2.5
1	B	158	ALA	2.5
1	B	39	SER	2.4
1	B	98	GLY	2.4
1	A	302	ALA	2.4
1	A	400	SER	2.3
1	B	429	ASN	2.3
1	A	420	ALA	2.3
1	A	325	LYS	2.3
1	B	375	THR	2.3
1	B	431	SER	2.3
1	B	157	HIS	2.2
1	B	404	ALA	2.2
1	A	237	GLU	2.2
1	A	125	ARG	2.1
1	A	262	SER	2.1
1	A	383	LEU	2.1
1	A	254	GLY	2.1
1	A	306	PHE	2.1
1	A	379	PHE	2.1
1	B	400	SER	2.0
1	A	34	VAL	2.0
1	A	272	GLY	2.0
1	A	219	ASN	2.0
1	A	384	VAL	2.0
1	B	418	ASP	2.0
1	B	403	LEU	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains

There are no non-standard protein/DNA/RNA residues in this entry.

### 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

### 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
4	TRS	A	460	8/8	0.76	0.23	1.46	55,58,60,60	0
3	PO4	B	442	5/5	0.88	0.17	-0.18	46,46,48,48	0
3	PO4	A	442	5/5	0.98	0.12	-1.11	32,32,35,35	0
2	MG	B	440	1/1	0.92	0.10	-1.20	29,29,29,29	0
2	MG	A	440	1/1	0.94	0.08	-1.97	39,39,39,39	0
2	MG	A	441	1/1	0.90	0.07	-2.84	38,38,38,38	0

### 6.5 Other polymers [i](#)

There are no such residues in this entry.